

# Matrix Decomposition By Additive and Subtractive Factors

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**Abstract**—A non-negative matrix factorization (NMF) is effectively applied to analyze data in an unsupervised way. Though non-negative factors are endowed with favorable interpretability, such as part-based representation, NMF lacks flexibility, being only applicable to data composed of non-negative values. In this paper, we propose a novel approach to enhance both flexibility and interpretability of matrix factorization. While NMF approximates a matrix in an additive form of non-negative factors, the proposed method disentangles the matrix into *additive* and *subtractive* parts by exploiting non-negative factors with a center factor akin to the average of data. Thereby, the disentanglement flexibly deals with any *real-valued* data beyond non-negative ones while rendering clear functionality to the factors. In the experiments on several factorization tasks using real-world data, the proposed method provides effective factorization to embed well interpretability especially into factors for analyzing intrinsic characteristics of the data.

**Index Terms**—matrix factorization, non-negativity, additive and subtractive form, interpretability.

## I. INTRODUCTION

While supervised learning renders discriminative models by using plenty of labeled samples [1], unsupervised approaches are effective for analyzing real-world data less annotated. To explore intrinsic characteristics of the data, the unsupervised methods can excavate *factors* that essentially constitute the data. Factor analysis is formulated based on such as statistical criteria in PCA and ICA [2] and physical constraints of *non-negativity* in non-negative matrix factorization (NMF) [3], [4].

In NMF, both factors and coefficients are defined as matrices composed of non-negative elements. Real-world signals are frequently acquired in a non-negative form through some physical measurement, such as image pixels. Accordingly, NMF is built upon the assumption that those non-negative signals are constructed by *addition* of non-negative factors which resemble parts [3]. Due to the non-negativity constraints, NMF facilitates data analysis [5], [6] through the interpretable factors of part-based representation in signals. To further increase interpretability of factors, regularization is additionally introduced into NMF, such as sparsity [7] and parametric representation [8]. NMF is also applied to cluster analysis of data distribution [9] and to deep framework [10].

A fundamental formulation of NMF is to reconstruct data by *adding* non-negative factors. While effective data analysis in NMF is attributed to the non-negative factors, the *additive* form is not so general to cover various physical characteristics found in real-world signals. Specifically, it is probable that

some factors work in a *subtractive* manner to describe data. For example, as in PCA, the average of signals is a central representation for the signal patterns, and thereby some samples are described by *subtracting* some factors from the average. In the other example, there are part-based factors described by *lower-intensity* signals in contrast to the others such as average and background signals; on face images, one can observe that hairs, eyes and beards are occasionally depicted by *dark* colors of low intensity. In an NMF framework, it is hard to describe those data by only *adding* non-negative factors from scratch, or it may require considerable amount of factors to describe it. Since those parts are missed in the additive non-negative factors, it is quite difficult to recognize the existence of those missing parts in NMF, degrading interpretability. Subtracting non-negative factors may also be related to semi-NMF [11] that frees coefficients from non-negativity constraints while retaining non-negative factors; those factors are added or subtracted according to real-valued coefficients. It, however, impedes interpretability of factors as they work in both ways of addition and subtraction in semi-NMF. Data analysis can be facilitated by identifying the functionality of factors, that is, whether the factor works in an additive or subtractive form.

In this study, we propose a novel factorization method to leverage non-negative factors to describe data for further increasing interpretability. We build a framework to decompose sample vectors into *additive* and *subtractive* parts by means of non-negativity constraints in conjunction with central representation (Fig. 1). In contrast to NMF, the proposed method can flexibly describe a sample vector not only by *addition* of some non-negative factors but also by *subtraction* of the other factors. Thereby, the method is applicable to *real-valued* signals beyond non-negative ones, while rendering clear functionality to the factors for enhancing interpretability.

## II. METHODS

### A. Matrix factorization

Suppose we have  $n$  samples of  $d$ -dimensional feature vector to form a matrix of  $\mathbf{X} \in \mathbb{R}^{d \times n}$ ; the features are *not* subject to non-negativity constraint but have *real* values. As in a standard factorization, the feature matrix  $\mathbf{X}$  is decomposed by

$$\mathbf{X} \approx \mathbf{W}\mathbf{H} \Rightarrow \min_{\mathbf{W}, \mathbf{H}} \|\mathbf{X} - \mathbf{W}\mathbf{H}\|_F^2, \quad (1)$$

where factors and coefficients are denoted by  $\mathbf{W} \in \mathbb{R}^{d \times r}$  and  $\mathbf{H} \in \mathbb{R}^{r \times n}$  with a prefixed rank  $r$ , respectively.

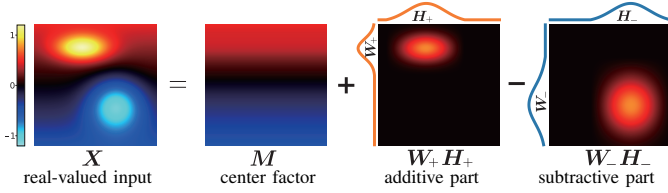


Fig. 1. Proposed matrix factorization. A *real-valued* matrix  $X$  is decomposed into additive and subtractive parts, with a baseline of a center factor  $M$ . In this case of rank  $r = 2$ , each of 1-rank non-negative parts,  $W_+H_+$  and  $W_-H_-$ , captures the intrinsic structure.

While (1) leads to singular-value decomposition through orthogonal constraints on the factors  $W$  and  $H$ , it is sophisticated by introducing non-negativity constraints [3], [4];

$$s.t. \mathbf{W} \geq 0, \mathbf{H} \geq 0, \quad (2)$$

where the inequality works on every element of a matrix, indicating all elements of  $W$  and  $H$  are *non-negative*. The constraint formulates non-negative matrix factorization (NMF) naturally rendering interpretable factors [3] *only if* the target data  $X$  are subject to non-negative constraint  $X \geq 0$ . Thus, it is hard to analyze a *real-valued* matrix as the non-negative factors only encode non-negative parts of  $X$  due to the non-negative coefficients  $H$  implying *addition* of factors.

On the other hand, semi-NMF [11] can exclude the non-negativity constraint from  $H$ . However, the relaxation degrades interpretability especially in terms of functionality of the non-negative factors  $W$ ; the  $i$ -th factor  $w_i$ , the  $i$ -th column vector of  $W$ , can work *inconsistently* in an additive or subtractive way depending on sign of the coefficient  $H_{ij} \in \mathbb{R}$ . Besides, the factors of semi-NMF are less localized as shown in Fig. 2 due to lack of constraints unlike NMF. Thus, semi-NMF is less interpretable for factor-based data analysis.

### B. Proposed formulation

We propose a method to decompose a *real-valued* matrix  $X \in \mathbb{R}^{d \times n}$  into *additive* and *subtractive* parts for enhancing both flexibility and interpretability, as shown in Fig. 1;

$$X \approx M + W_+H_+ - W_-H_-, \quad (3)$$

where we introduce a *real-valued* center factor  $M \in \mathbb{R}^{d \times n}$  and *non-negative* factors  $W_+, W_-, H_+$  and  $H_-$  of rank  $\frac{r}{2}$ ; it is practically possible to assign different ranks to the additive and subtractive factors, though the uniform rank  $\frac{r}{2}$  works well in the experiments (Sec. III).

While the center factor  $M$  works as a baseline, the *additive* and *subtractive* parts are given as  $W_+H_+$  and  $W_-H_-$ , respectively. Due to the non-negativity, those factors retain the interpretability as in NMF, i.e., part-based representation. (3) is a general formulation of NMF since it is reduced into non-negative factorization in case of  $X \geq 0$  and  $M = 0$ . It is also noteworthy that even for non-negative target  $X \geq 0$ , both additive and subtractive parts contribute to analyzing the target by capturing deviation patterns from the baseline pattern  $M \geq 0$ . Thus, the proposed decomposition (3) renders flexible analysis by exploring diverse factors of the target pattern data.

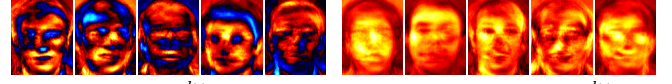


Fig. 2. Factors  $W$  produced by two types of semi-NMF for ORL faces [12]. These factors can be compared with those of NMF and ours in Fig. 4(a,b).

To effectively optimize those factors, our factorization in (3) leads to the optimization problem of

$$\min_{\mathbf{W} \geq 0, \mathbf{H} \geq 0, M} \|\mathbf{X} - \mathbf{M} - \mathbf{W}\mathbf{J}\mathbf{H}\|_F^2 + \lambda\Omega(\mathbf{W}, \mathbf{H}), \quad (4)$$

where  $\mathbf{J} = \text{blkdiag}(\mathbf{I}, -\mathbf{I}) \in \mathbb{R}^{r \times r}$  using an identity matrix  $\mathbf{I}$ ,

$$\mathbf{W} = [\mathbf{W}_+, \mathbf{W}_-] \in \mathbb{R}_+^{d \times r}, \mathbf{H} = [\mathbf{H}_+^\top, \mathbf{H}_-^\top]^\top \in \mathbb{R}_+^{r \times n}. \quad (5)$$

The formulation contains a regularization  $\Omega$  with a weight parameter  $\lambda$ , which is detailed in the next section.

### C. Regularization

While a standard NMF incorporates factor-wise regularization [13], we formulate the regularization  $\Omega(\mathbf{W}, \mathbf{H})$  as

$$\begin{aligned} \Omega(\mathbf{W}, \mathbf{H}) &= \|\mathbf{W}_+H_+\|_F^2 + \|\mathbf{W}_-H_-\|_F^2 + 2\langle \mathbf{W}_+H_+, \mathbf{W}_-H_- \rangle \\ &= \|\mathbf{W}_+H_+ + \mathbf{W}_-H_-\|_F^2 = \|\mathbf{W}\mathbf{H}\|_F^2. \end{aligned} \quad (6)$$

The first two terms are  $L_2$ -regularization on additive and subtractive parts for enhancing robust and stable representation. In contrast to regularized NMF [13] which applies  $L_2$ -regularization to respective factors  $W$  and  $H$ , our regularization works in a part-wise manner for  $W_+H_+$  and  $W_-H_-$  since we focus on disentanglement of the positive and negative parts. Besides, it also regularizes norm of respective factors via

$$\|\mathbf{W}_+H_+\|_F^2 = \text{tr}(\mathbf{W}_+H_+H_+^\top\mathbf{W}_+^\top) = \langle \mathbf{W}_+, \mathbf{W}_+ \rangle_{H_+H_+^\top},$$

where  $\text{tr}$  is a trace operator. It indicates norm of factors  $W_+$  embedded by the positive semi-definite matrix  $H_+H_+^\top$ . Thus, the first two terms in (6) work as regularization for both part-based and factor-based representation.

The third term  $\langle \mathbf{W}_+H_+, \mathbf{W}_-H_- \rangle$ , an inner product between  $W_+H_+$  and  $W_-H_-$ , contributes to reducing overlap of those two parts by promoting  $(\mathbf{W}_+H_+) \odot (\mathbf{W}_-H_-) \rightarrow \mathbf{0}$ . Overlapped additive and subtractive parts are redundant to impede compactness and interpretability in factorization.

The above-mentioned two kinds of regularization are unified into a simple form of  $\|\mathbf{W}\mathbf{H}\|_F^2$  in (6), though it is also possible to trivially inject  $\|\mathbf{W}_+\|_F^2$  and  $\|\mathbf{W}_-\|_F^2$  into  $\Omega$ .

### D. Center factor M

We apply an *affine* approach to model the center factor  $M$ ;

$$M = \mu\mathbf{a}^\top + \mathbf{1}\mathbf{b}^\top \in \mathbb{R}^{d \times n}, \quad (7)$$

which contains three types of trainable parameters,  $\mu \in \mathbb{R}^{d \times 1}$ ,  $\mathbf{a} \in \mathbb{R}^{n \times 1}$  and  $\mathbf{b} \in \mathbb{R}^{n \times 1}$ . Generally speaking, each feature vector  $x_i$  could have its own center representation in an affine model of  $a_i\mu + b_i\mathbf{1}$  on the basis of global mean representation  $\mu$  shared across all samples. Scaling factor  $a_i$  and bias  $b_i$  cope with sample-wise variation such as illumination changes in image data and common dynamics patterns in temporal signal data. Thereby, (7) encodes a complicated center factor  $M$ .

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**Algorithm 1** Proposed method

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**Input:**

$\mathbf{X} \in \mathbb{R}^{d \times n}$ : input matrix,  $r$ : number of factors,  
 $\mathbf{M}$ : center factor (7) initialized by using  $\hat{\mathbf{X}} = \mathbf{X}$  in (10),  
 $\mathbf{W} \sim \mathcal{U}[0, 1]^{d \times r}$ ,  $\mathbf{H} \sim \mathcal{U}[0, 1]^{r \times n}$ : randomly initialized  
non-negative matrices via uniform distribution on  $[0, 1]$ ,  
 $\epsilon$ : small tolerance for convergence

1: **repeat**

2: Optimize  $\mathbf{W}$  and  $\mathbf{H}$  while fixing  $\mathbf{M}$  by applying  
Nesterov method [14] in (9).

3: Optimize  $\mathbf{M}$  while fixing  $\mathbf{W}$  and  $\mathbf{H}$  by (10).

4: **until** Gradient magnitude w.r.t  $\mathbf{W}$  and  $\mathbf{H}$  are less than  $\epsilon$

**Output:**  $\mathbf{W}, \mathbf{H}, \mathbf{M}$ : optimal factors for  $\mathbf{X} \approx \mathbf{M} + \mathbf{W}\mathbf{J}\mathbf{H}$ .

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### E. Optimization

We derive the following objective loss from (4, 6),

$$J(\mathbf{W}, \mathbf{H}, \mathbf{M}) = \|\mathbf{X} - \mathbf{M} - \mathbf{W}\mathbf{J}\mathbf{H}\|_F^2 + \lambda \|\mathbf{W}\mathbf{H}\|_F^2. \quad (8)$$

As in the other NMF methods, it is a non-convex function, for which it is hard to attain global minimizer. Therefore, toward effective optimization, we apply an alternative approach with respect to three variables of  $\mathbf{W}$ ,  $\mathbf{H}$  and  $\mathbf{M}$ , which is detailed as follows; the optimization process is summarized in Alg. 1.

**Optimization w.r.t  $\mathbf{W}$  and  $\mathbf{H}$ :** This is similar to least-square minimization for the target matrix  $\hat{\mathbf{X}} = \mathbf{X} - \mathbf{M}$  with non-negativity constraints regarding  $\mathbf{W}$  and  $\mathbf{H}$ . Thus, following the optimization approach in NeNMF [14], it is efficiently optimized by Nesterov's optimal gradient method [15] to iteratively optimize  $\mathbf{W}$  and  $\mathbf{H}$ . Given the  $t$ -th optimizer  $\hat{\mathbf{W}}$ , the optimization problem w.r.t  $\mathbf{H}$  is formulated as

$$\mathbf{H}^{t+1} = \arg \min_{\mathbf{H} \geq 0} J_H(\mathbf{H}), \quad (9)$$

$$J_H(\mathbf{H}) = \text{tr}[\mathbf{H}^\top (\hat{\mathbf{W}}^\top \hat{\mathbf{W}} + \mathbf{J}^\top \hat{\mathbf{W}}^\top \hat{\mathbf{W}} \mathbf{J}) \mathbf{H} - 2\mathbf{H}^\top (\mathbf{J}^\top \hat{\mathbf{W}}^\top \hat{\mathbf{X}})].$$

It satisfies the two conditions required for the Nesterov method [14] that (i)  $J_H(\mathbf{H})$  is convex and (ii) the derivative  $\nabla J_H(\mathbf{H})$  is Lipschitz continuous; these are proved by directly applying the proof of Lemma 1&2 in [14].

**Optimization w.r.t  $\mathbf{M}$ :** Then, the center factor  $\mathbf{M}$  is optimized by means of least squares in which the target is defined as a residual  $\tilde{\mathbf{X}} = \mathbf{X} - \mathbf{W}\mathbf{J}\mathbf{H}^\top$ , based on a model (7) without regularization regarding  $\Omega$ . Thus, the optimizer of the center factor  $\mathbf{M}$ , parameterized by  $\mathbf{a}$ ,  $\mathbf{b}$  and  $\boldsymbol{\mu}$  in (7), is given by

$$\mathbf{b}^* = \frac{1}{d} \tilde{\mathbf{X}}^\top \mathbf{1}_d, \quad (\boldsymbol{\mu}^*, \mathbf{a}^*) = \text{svd}_1(\tilde{\mathbf{X}} - \mathbf{1}\mathbf{b}^\top), \quad (10)$$

where  $\text{svd}_1$  indicates a 1-rank SVD operation which is efficiently computed by power iteration [16] or conjugate gradient [17]; let  $\tilde{\mathbf{X}} - \mathbf{1}\mathbf{b}^\top \approx \mathbf{u}\mathbf{sv}^\top$  be 1-rank SVD, and then we have  $\boldsymbol{\mu}^* = \sqrt{s}\mathbf{u}$  and  $\mathbf{a}^* = \sqrt{s}\mathbf{v}$ .

## III. RESULTS

We apply the proposed method to various factorization tasks, lower-dimensional feature representation, image factorization and stock data analysis; datasets used in these

experiments are summarized in Table I. It is evaluated in comparison to NeNMF [14], sophisticated non-negative factorization. For fair comparison, we perform factorization with the same number of rank  $r$  for ours and NeNMF, as shown in Table II; in our method,  $r$  factors are equally divided into additive and subtractive parts. We set a regularization weight by  $\lambda = 0.01$  in (4), while NeNMF is similarly equipped with  $L_2$  regularization using the same weight, for fair comparison.

### A. Lower-dimensional feature representation

The methods are quantitatively evaluated on a task of compressing feature vectors using the datasets of multi-feature [18] and Isolet [19], which are detailed in Table I. Through factorization (1, 4), a feature matrix  $\mathbf{X} \in \mathbb{R}^{d \times n}$  is represented in a lower-dimensional latent space of the coefficients  $\mathbf{H} \in \mathbb{R}_+^{r \times n}$ . In this clustering task, for reference, we additionally apply semi-NeNMF which relaxes the non-negativity constraint on the factors in NeNMF to produce  $\mathbf{W} \in \mathbb{R}^{d \times r}$  and  $\mathbf{H} \in \mathbb{R}_+^{r \times n}$ . To evaluate the lower-dimensional representation, we measure normalized mutual information (NMI) through k-means clustering in the space with a ground-truth class labels (Table I).

Table III shows performance results, demonstrating the efficacy of the proposed method over NMFs. Our method well extracts discriminative representation by considering additive and subtractive deviation from a center factor to effectively encode detailed characteristics of features.

### B. Face image factorization

We then apply the methods to factorize face images of *non-negative* pixels into parts on ORL [12] and AR [20] face datasets (Table I). The estimated factors  $\mathbf{W}$  are shown in Fig. 4 for ORL and AR datasets, respectively, exhibiting part-based representation of face; semi-NMF fails to extract part-based factors as shown in Fig. 2. While NeNMF extracts factors solely operating in an additive manner, our method provides two types of additive and subtractive factors in terms of pixel values. Thus, additive factors represent relatively *brighter* components and negatives ones correspond to *darker* components, such as *eye* and *beard* regions. It leads to semantically separable parts, while NeNMF detects rather entire skin parts.

The methods are also quantitatively evaluated by sparsity of

$$\text{sparsity}(\mathbf{W}) = |\{W_{ij} | W_{ij} = 0\}_{i=1, j=1}^{d, r}| / (d \cdot r). \quad (11)$$

As shown in captions of Fig. 4, our factors exhibit higher sparsity scores as well as better NMI. Thus, while extracting the discriminative characteristics, our method provides sparse factors which provide compact part-based representation.

### C. Stock data analysis

Finally, the factorization method is applied to analyze real-world data which are equipped with no supervised annotation. We focus on data of share price movements which would contain some factors (movement tendency) across several stocks. We constructed a stock price dataset by picking up 162 stocks included in Nikkei-225, a representative index in the Japanese stock market, and sampled the opening, closing,

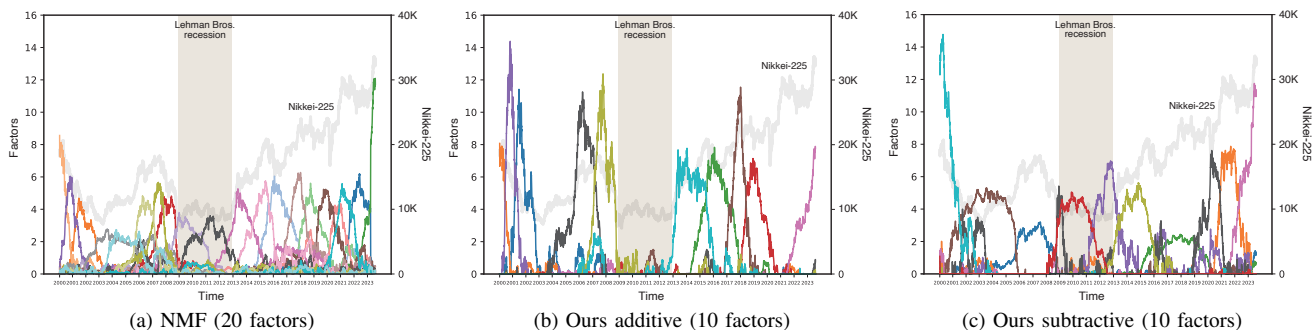


Fig. 3. Factors on the stock-price dataset. This shows 20 factors on each method, with Nikkei-225 index (light-gray line). (a) NeMF produces 20 non-negative factors. Our method provides (b) 10 positive and (c) negative factors, respectively, to provide 20 factors in total. Best viewed in color.

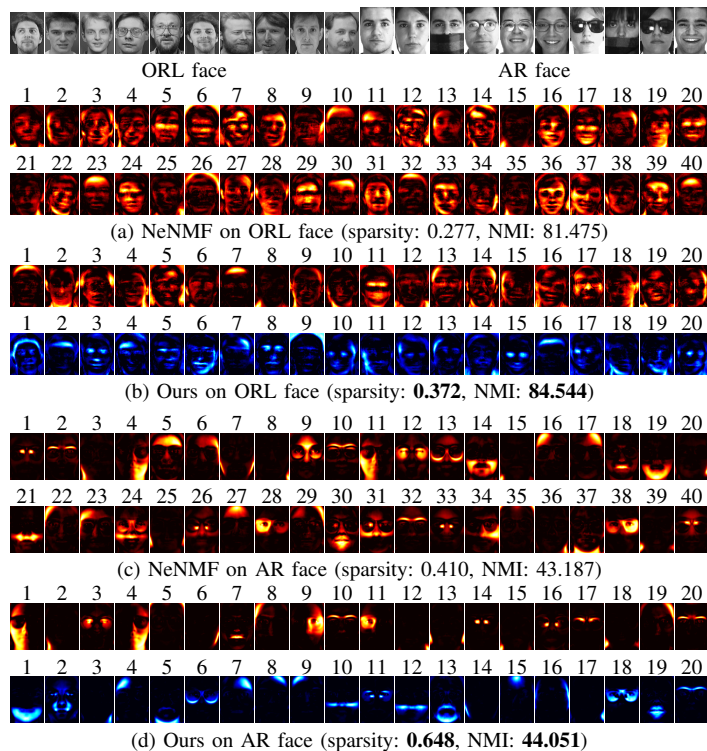


Fig. 4. Visualization of 40 factors for face images. Our method produces 20 additive and 20 subtractive factors shown in top and bottom rows, respectively. The sparsity score is also shown in sub-captions. This is best viewed in color.

high and low prices in the daily chart for each stock from Jan 4, 2000 to Aug 3, 2023 (5738 days). As a result, we collected 162 samples of 5738-dimensional *non-negative* feature vector by averaging the daily-chart prices. In the center factor (7), we prefix the mean vector  $\mu$  to the Nikkei-225 prices for enhancing interpretability; it is beneficial to embed such prior knowledge into our model especially through the center factor.

Fig. 3 shows the estimated factors on the stock data. The factors exhibit clear difference between ours and NeMF. In the proposed method, additive factors effectively describe the tendency that the stock price increases. Interestingly, one can find distinctive patterns of the additive factors that they are deactivated in a specific period from December 2008 to December 2012, which corresponds to the period of the economic recession after the collapse of Lehman Brothers [21]. As its counterpart, there is one negative factor that activates only

TABLE I  
DATASETS

Dataset	# sample ( $n$ )	# dimension ( $d$ )	# class
multi-feature [18]	2,000	649 features	10
Isolet [19]	7,797	617 features	26
ORL face [12]	400	$92 \times 112$ pixels	40
AR face [20]	2,600	$120 \times 165$ pixels	100
Stock price data	162	5738 days	-

TABLE II  
NUMBER OF FACTORS (RANK  $r$ )

	NeMF	Ours	
		Additive	Subtractive
multi-feature	20	10	10
Isolet	52	26	26
ORL face	40	20	20
AR face	40	20	20
Stock price data	20	10	10

TABLE III  
NORMALIZED MUTUAL INFORMATION (NMI)

	rate of non-negative feature elements	NMI		
		NeMF	semi-NeMF	Ours
multi-feature	(0.95)	77.200	61.470	<b>80.380</b>
Isolet	(0.58)	65.122	63.755	<b>70.615</b>

in this recession period. On the other hand, all the factors in NeMF are entangled to each other, making it hard to understand/interpret them for analyzing the stock data in detail.

The experimental result shows that our method facilitates data analysis by disentangling factors into additive and subtractive parts of better interpretability. By delving deep into the factors of clear functionality, we could further analyze essential phenomena embedded in data with semantic interpretation.

#### IV. CONCLUSION

We have proposed a novel factorization method to enhance both flexibility and interpretability. In contrast to NMF, our method models a matrix by using two types of factors working in additive and subtractive ways with a baseline of a central representation (factor). Thereby, it effectively extracts intrinsic characteristics of data, being flexibly applicable to any *real-valued* matrices as well as clarifying the functionality of factors to enhance interpretability. On several factorization tasks using real-world data, the proposed method exhibits favorable empirical performance and interpretability in contrast to NMF.

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